Fractional spinonic excitations in a 1D quantum antiferromagnet

$\text{SrCo}_2\text{V}_2\text{O}_8$

Zhe Wang
University of Augsburg

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TRR 80
From Electronic Correlations to Functionality

EMFL
European Magnetic Field Laboratory
* Experimental techniques: THz/Infrared spectroscopy
  * Quantum spin-dimer system

* 1D spin-1/2 Ising-like XXZ antiferromagnet SrCo$_2$V$_2$O$_8$
  * Realization of spinon confinement [PRB 91, 140404(R) (2015)]
  * Tuning the spinon excitations by external magnetic fields
Spin-1/2 dimer: singlet and triplet

- **Spin gap** \( \Delta = J_0 \)
- **Ground state**: spin singlet state
- **Excited state**: spin triplet state
- **Cr\(^{5+}\)**: 3d\(^1\), \( S = 1/2 \)
- **Monoclinic**
- **Spin dimer**
- **Singlet-triplet**

\[ J_0 \mathbf{S}_1 \cdot \mathbf{S}_2 \]

\( J_0 > 0 \): antiferromagnetic
Zeeman splitting

\[ J_0 \mathbf{S}_1 \cdot \mathbf{S}_2 + g \mu_B H (S_1 + S_2)^z \]

\( J_0 > 0 \): antiferromagnetic

Excited state: spin triplet state

Spin gap \( \Delta = J_0 \)

Ground state: spin singlet state

Zeeman term

\[ |S, S_z\rangle \]

\[ |1, +1\rangle \]

\[ |1, 0\rangle \]

\[ |1, -1\rangle \]

Intra-triplet

\[ |0, 0\rangle \]
Magnetic excitations

Selection rules:

Intra-triplet mode: \( h\omega \perp H \)

\( \Delta S = 0, \quad \Delta S_z = \pm 1 \)

- Conservation of \( S \)
- Magnetic-dipole active

**Singlet-triplet mode**

\( \Delta S = 1 \)

Violation of \( S \) conservation!

\( \rightarrow \) Dzyaloshinskii-Moriya interaction

\( D \cdot (S_1 \times S_2) \)

spin-orbit coupling
Symmetry and selection rule

$\text{Ba}_3\text{Cr}_2\text{O}_8$

$D = 0$

Inversion center

T. Moriya, Phys. Rev. 120, 91 (1960)
Symmetry and selection rule

$\text{Ba}_3\text{Cr}_2\text{O}_8$

*Dynamic* Dzyaloshinskii-Moriya: instantaneously symmetry broken due to optical phonons

$$
\sum_{i,\alpha,\beta} E_i^{\omega} A_{\alpha\beta} (S_{i1} \times S_{i2})_{\beta}
$$

Symmetry and selection rule

Every symmetry operation associates a dimer in one layer to another dimer in the neighboring layer.

$$ T_{12} \equiv S_1 \times S_2 $$

- $T_{12}^a \rightarrow T_{1'2'}^a$, $q=0$ in-phase mode
- $T_{12}^b \rightarrow -T_{1'2'}^b$, $q=\pi$ anti-phase mode

Selection rule

<table>
<thead>
<tr>
<th>$E^\omega \setminus H$</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a$</td>
<td>$0(A_{ab}) + \pi(A_{ac})$</td>
<td>$\pi(A_{aa}, A_{ac})$</td>
<td>$0(A_{ab}) + \pi(A_{aa})$</td>
</tr>
<tr>
<td>$b$</td>
<td>$0(A_{bc}) + \pi(A_{bb})$</td>
<td>$0(A_{ba}, A_{bc})$</td>
<td>$0(A_{ba}) + \pi(A_{bb})$</td>
</tr>
<tr>
<td>$c$</td>
<td>$0(A_{cb}) + \pi(A_{cc})$</td>
<td>$\pi(A_{ca}, A_{cc})$</td>
<td>$0(A_{cb}) + \pi(A_{ca})$</td>
</tr>
</tbody>
</table>
Experimental results: selection rule and spin-phonon coupling

Ba$_3$Cr$_2$O$_8$

<table>
<thead>
<tr>
<th>$E^o \setminus H$</th>
<th>$a_h$</th>
<th>$b_h$</th>
<th>$c_h$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_h$</td>
<td>$0 + \pi$</td>
<td>[Fig. 2(c), 3(b)]</td>
<td></td>
</tr>
<tr>
<td>$b_h$</td>
<td>$0 + \pi$</td>
<td>[Fig. 3(c)]</td>
<td></td>
</tr>
<tr>
<td>$c_h$</td>
<td>$0 + \pi$</td>
<td>[Fig. 3(d)]</td>
<td></td>
</tr>
</tbody>
</table>

**Dynamical** Dzyaloshinskii-Moriya interactions enabled instantaneously due to optical phonons

spin-phonon coupling

ZW et al, PRB 89, 174406 (2014) with O. Cépas, S. Zvyagin
* Powerful technique for investigating magnetic interactions and dynamics
  characteristic energy range of 1 - 100 meV (THz and FIR spectral range)

* Various tunable parameters:
  • Polarization  → selection rules, anisotropies → symmetry
  • Magnetic field  → exchange interactions/anisotropies
    → spin hamiltonian
    → classical/quantum phase transitions
    → emergent phenomena
  • Temperature  → phase transitions, thermal fluctuations
  • ……
THz time-domain spectroscopy (THz-TDS)

Spectral range: 1 – 16 meV (0.25 – 4 THz)

Temperature range: 4.2 – 300 K

TeraView Ltd
High-field electron spin resonance (ESR) transmission spectroscopy

### Optical Table Diagram

- **Source (BWOs)**
- **Detector**
- **f**: 0.1-1.4 THz (monochromatic)
- **$e^i$**: polarization
- **$H$**: 7 T
- **$e^o$**: polarization
- **2 – 300 K**
High-field Fourier transform infrared spectroscopy (FTIR)

Michelson interferometer

Bitter magnet (32T)

Bruker Optik

1.5 – 300 K

© HFML Nijmegen
Outline

* Experimental techniques: THz/Infrared spectroscopy
  * Quantum spin-dimer system

* 1D spin-1/2 Ising-like XXZ antiferromagnet SrCo$_2$V$_2$O$_8$
  * Realization of spinon confinement
  * Tuning the spinon excitations by external magnetic fields
Crystalline and magnetic structure of $\text{SrCo}_2\text{V}_2\text{O}_8$

- Tetragonal structure
- Screw chain along the $c$ axis
- Edge-sharing CoO$_6$ octahedra
- 4 Co$^{2+}$ ions per unit cell

![Diagram of SrCo$_2$V$_2$O$_8$ structure]

Energy levels for Co$^{2+}$ (3$d^7$):
- $^4P$
- $^4A_2$
- $^4F$ ($I = 3, s = 3/2$)
- $^4T_2$
- $^4T_1$ ($I \approx 1, s = 3/2$)

- Free ion
- Cubic field
- Spin-orbit coupling

$\tilde{S} = 5/2$
$\tilde{S} = 3/2$
$\tilde{S} = 1/2$
Crystalline and magnetic structure of $\text{SrCo}_2\text{V}_2\text{O}_8$

1. Realization of the 1D XXZ spin-1/2 model

\[ J \sum_i \left[ S_i^z S_{i+1}^z + \epsilon (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \right] \]

- \( J > 0 \)
- Antiferromagnetic nearest-neighbor exchange interaction

\[ 0 < \epsilon < 1 \]
- Ising-like exchange anisotropy

Longitudinal: parallel to the z direction (along the c axis)

Transverse: perpendicular to the z direction (along the a axis)

Crystalline and magnetic structure of SrCo$_2$V$_2$O$_8$

2. Interchain coupling:
   • 3D Néel antiferromagnetic ordering below $T_N \sim 5\text{K}$

Neutron diffraction:

$J'/J < 10^{-2}$
Spinon confinement in 1D Ising-like antiferromagnet
Spinon excitations of Ising chain

Ising antiferromagnetic spin-1/2 chain

One spin flip $\rightarrow$ Two spinons

$$\Delta S^z = \pm 1$$

$$E = J$$

Highly degenerate excited states
Spinon excitations of XXZ chain

Ising-like (XXZ) spin-$1/2$ antiferromagnetic chain

\[ J \sum_{i=1}^{N} [S_i^z S_{i+1}^z + \epsilon(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)] \]

\[ 0 < \epsilon < 1 \text{ (Ising-like)} \]

Parabolic dispersion relation
(close to the $\Gamma$ point, approximate)

Interchain exchange interaction: confinement potential

$T < T_N$

Two-spinon bound states

$J'$: interchain coupling

1D Schrödinger equation of two-spinon bound states

One-dimensional Schrödinger equation:

\[-\frac{\hbar^2}{\mu} \frac{d^2 \varphi}{dz^2} + \lambda |z| \varphi = (E - 2E_0) \varphi\]

Solution:

\[E_j = 2E_0 + \zeta_j \lambda^{2/3} \left( \frac{\hbar^2}{\mu} \right)^{1/3}\]

\(\zeta_j\) are the negative zeros of the Airy function

Linear dependence:
Characteristics of confined spinons

Result I: Realization of spinon confinement
Spinon absorption spectra

**THz Time domain signal**

**Frequency domain signal**

SrCo$_2$V$_2$O$_8$

$T_N \sim 5K$

Fourier Transform

ZW et al PRB 91, 140404(R) (2015)
Spinon absorption spectra

Series of excitations:
- Below $T_N$ : magnetic order

Characteristic features:
- Energy increases
- Intensity decreases
- Energy difference decreases

$T_N \sim 5\text{K}$

$\text{SrCo}_2\text{V}_2\text{O}_8$

ZW et al PRB 91, 140404(R) (2015)
Series of confined spinons

One-dimensional Schrödinger equation with linear confinement potential:

$$-\frac{\hbar^2}{\mu} \frac{d^2 \varphi}{dz^2} + \lambda |z| \varphi = (E - 2E_0) \varphi$$

Solution:

$$E_j = 2E_0 + \zeta_j \lambda^{2/3} \left( \frac{\hbar^2}{\mu} \right)^{1/3}$$

$\zeta_j$ are the negative zeros of the Airy function

Discussion: selection rule

- Two-spinon bound state $S = \pm 1$: odd number of spin flips
- Two-spinon bound state $S = 0$: even number of spin flips

both series observed by neutron scattering

Result II: magnetic-field tuning

*Longitudinal* magnetic field
... in a *longitudinal* magnetic field

High-field ESR \( H \parallel z \)

\[
\text{SrCo}_2\text{V}_2\text{O}_8 \quad T < T_N
\]

ZW et al PRB 91, 140404(R) (2015)
… in a *longitudinal* magnetic field

High-field ESR $H \parallel z$

Linear field dependence described by a single Zeeman term

$$\pm g_\parallel \mu_B H S$$

$g_\parallel = 5.5 \quad S = 1$

(Distortion of CoO$_6$ octahedra)

ZW et al PRB 91, 140404(R) (2015)
Split of bound states in longitudinal magnetic field

\[ H \parallel z \]

- Higher-energy confined spinons determined from linear extrapolation of field dependence
- Two-spinon bound state doubly degenerate at zero field and split in finite longitudinal field
- Two-spinon bound state \( S = \pm 1 \)

\[ E_j = 2E_0 + \zeta_j \chi^{2/3} \left( \frac{\hbar^2}{\mu} \right)^{1/3} \]

ZW et al PRB 91, 140404(R) (2015)
4-spinon continuum, excitations of the critical spin-liquid phase, etc

- Two pairs of bound-spinons continuum to be checked (e.g. linewidth)?
- Excitations in the critical region?
- Field dependence in BaCo$_2$V$_2$O$_8$
Result II: magnetic-field tuning

Transverse magnetic field
in the antiferromagnetic phase

\[ H \parallel x \quad T < T_N \]

ZW et al, unpublished
in the antiferromagnetic phase

One-dimensional Schrödinger equation with linear confinement potential:

\[-\frac{\hbar^2}{\mu} \frac{d^2 \varphi}{dz^2} + \lambda |z| \varphi = (E - 2E_0)\varphi\]

\[E_j = 2E_0 + \zeta_j \lambda^{2/3} \left( \frac{\hbar^2}{\mu} \right)^{1/3}\]

ZW et al, unpublished
in the antiferromagnetic phase

\[ E_j = 2E_0 + \zeta_j \lambda^{2/3} \left( \frac{\hbar^2}{\mu} \right)^{1/3} \]
in the antiferromagnetic phase

\[ E_j = 2E_0 + \zeta_j \lambda^{2/3} \left( \frac{\hbar^2}{\mu} \right)^{1/3} \]
Low temperature phase diagram of \( \text{BaCo}_2\text{V}_2\text{O}_8 \) in transverse magnetic fields

\( \text{BaCo}_2\text{V}_2\text{O}_8 \): critical field \( H_c \sim 9 \text{ T} \) at 1.5K

\( \text{SrCo}_2\text{V}_2\text{O}_8 \): critical field \( H_c \sim 7 \text{ T} \) at 1.5K

S. K. Niesen, Th. Lorenz et al. PRB 87, 224413 (2013)
in the disordered phase

\[ H \parallel x \]

Field dependence:

- \( \alpha \) evolves from confined spinons
- \( \beta_+ , \beta_- \) are degenerate at zero field and split in finite field
- \( \alpha, \beta_- \) avoid crossing at high fields above \( 22T \)

ZW et al, unpublished
Summary

* Observation of confined spinon excitations in the 1D XXZ antiferromagnet SrCo$_2$V$_2$O$_8$
  → linear confinement potential by interchain coupling
  → described by one-dimensional Schrödinger equation
* Tuning of spinon excitations by magnetic fields
  Longitudinal magnetic field
  → linear dependence in the ordered phase
  Transverse magnetic field
  → non-linear field dependence